

Correlations, Plasmarons, and Quantum Spectral Function in Bilayer Graphene

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We theoretically study the many-body effects of electron-electron interaction on the single particle spectral function of doped bilayer graphene. Using random phase approximation, we calculate the real and imaginary part of the self-energy and hence the spectral function. The spectral function near the Fermi surface shows the usual quasiparticle peak, establishing doped bilayer graphene, in contrast to the unstable neutral system, to be a Fermi liquid. Away from the Fermi surface, an additional broad plasmaron peak is visible in the spectral function. From the low energy behaviour of the self-energy we calculate the quasiparticle residue and the effective mass of the quasiparticles as a function of carrier density. We present results for both the on-shell and the off-shell approximation for the quasiparticle renormalization.

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Bilayer graphene (BLG) has attracted both experimental and theoretical interest as a novel 2D gapless chiral electron-hole system with parabolic dispersion [1], where carrier density can be easily tuned by applying a gate voltage. From a many-body interaction physics perspective, BLG is particularly intriguing as it lies between the chiral and gapless single layer graphene (SLG), which has linear band dispersion, and 2D semiconductor-based electron gas (2DEG) systems, which are non-chiral and gapped, but typically have quadratic band dispersion [2]. In addition, the interaction parameter in BLG can be simply tuned by changing the carrier density whereas in SLG the interaction parameter is the fine structure constant which is fixed for a given substrate. BLG is therefore the ideal system to study chiral interaction physics since interaction effects in SLG are typically small [1]. It is therefore quite surprising that very little BLG interaction physics has so far been studied in the literature, perhaps because of serious technical difficulties of treating both intraband and interband virtual processes on an equal footing in a gapless system. In this Letter we provide the first theoretical treatment of the many-body interaction effects on the BLG single-particle properties as a function of carrier density. Our work, being directly comparable to experimental data, should motivate experimental studies of BLG many-body properties.

An important many-body property of BLG is the single particle spectral function $A(\mathbf{k}, \omega)$, which measures the probability of finding an electron (hole) with a momentum \mathbf{k} and energy ω in the system (We take $\hbar = 1$ throughout.) The spectral function, which gives detailed information about electronic structure and many-body renormalization, can be measured by angle resolved photo-emission spectroscopy (ARPES) [3]. In the absence of interaction, the spectral function is simply a delta function giving the non-interacting band energy at momentum \mathbf{k} . The modification of the spectral function due to electron-electron interactions is a matter of great interest both theoretically and experimentally. A pressing question in this respect is whether BLG behaves like a Fermi liquid, where phase space restrictions near the Fermi surface lead to sharply

defined quasiparticles with a finite spectral weight.

In this letter, we calculate the carrier density dependent single particle spectral function of doped BLG, taking into account electron-electron interactions within the dynamical random phase approximation (RPA). We find that the BLG spectral function has a broad plasmaron peak, i.e. a peak associated with the quasiparticle carrying a cloud of virtual plasmons, in addition to the Landau quasiparticle peak. We obtain the quasiparticle renormalization and the effective mass, which completely define the low energy coherent part of the spectral function around the Fermi surface, and study their variation with the carrier density. We find that quasiparticle spectral weight decreases with decreasing density while the effective mass shows a non-monotonic behaviour. The effective mass remains smaller than the bare mass down to relatively low densities with a maximum renormalization of $\sim 20\%$, thus showing that the system remains a weakly interacting Fermi liquid even at low densities. Earlier BLG many-body theoretical work restricted itself [4] to either Hartree-Fock or static screening theories neglecting dynamical correlations, which is known to be inadequate in interacting electron systems where dynamical screening is important.

A key question for BLG, indeed for any electronic material, is whether the presence of interaction preserves the Fermi liquid behavior, where the system manifests one-to-one correspondence with the noninteracting system in its low-energy properties, or leads to an exotic non-Fermi liquid. This question has recently been addressed [5] in the literature for neutral undoped BLG which exists only at the Dirac point. Not surprisingly such a pure zero-density Fermi system is found to be a non-Fermi-liquid in the presence of interaction. We show in the current work that this Dirac point non-Fermi liquid behavior of neutral BLG is unstable to the existence of any finite doping, and doped BLG is always a Fermi liquid in the presence of any finite carrier density (which is always true in any physical BLG system). Our finding that the BLG is a Fermi liquid similar to regular non-chiral 2DEG systems is directly experimentally verifiable through ARPES since the singularity structure of the theoretical spectral function is very different in the doped and the undoped situations. We find that

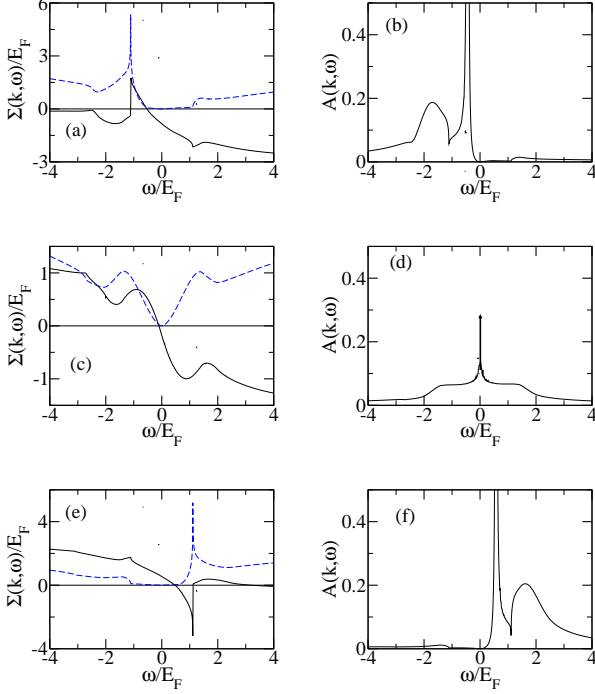


FIG. 1: (Color online) Left column: The real (thick black line) and imaginary part (dashed blue line) of self-energy for (a) $k = 0.75k_F$, (c) $k = k_F$ and (e) $k = 1.25k_F$. The absolute value of the imaginary part is plotted in these graphs. Right column: Single particle spectral function for the same wave vectors, (b) $k = 0.75k_F$, (d) $k = k_F$ and (f) $k = 1.25k_F$. The system is characterized by $r_s = 3$. The Dirac point is at $\omega = -E_F$.

the neutral non-Fermi liquid fixed point is an unstable set of measure zero, which will always become a Fermi liquid fixed point in the presence of density fluctuations. This is an important new result since density fluctuations are invariably present in all real BLG samples due to thermal and disorder effects.

We work with the low energy two band parabolic approximation to the BLG Hamiltonian where the dispersions of the bands are given by $E_{s\mathbf{k}} = s^2 k^2 / 2m_0$ where $s = \pm 1$ denotes the conduction and valence bands and m_0 is the non-interacting BLG mass with $m_0 \simeq 0.033m_e$, m_e being the mass of a free electron. The chiral band wave functions are given by $\psi_{s\mathbf{k}}^\dagger = (e^{i2\theta_{\mathbf{k}}}, s) / \sqrt{2}$, where $\theta = \tan^{-1}(k_y/k_x)$ is the azimuthal angle in the momentum space. Each band has a degeneracy factor of $g = 4$ (2 for spin and 2 for valley). We note that the 2-band parabolic BLG approximation is well-justified because we are interested in the low-energy behavior, and at high doping densities, where the parabolic approximation fails, the BLG dispersion becomes linear with the system behaving like the SLG whose many-body properties have already been studied in the literature [1, 6].

The non-interacting Green function for the system is given by $G_0(s, \mathbf{k}, \omega) = (\omega - \xi_{s\mathbf{k}})^{-1}$, where $\xi_{s\mathbf{k}} = E_{s\mathbf{k}} - E_F$ with E_F being the Fermi energy. The corresponding spectral function consists of delta function peaks at the

band dispersion energies and is given by $A_0(s, \mathbf{k}, \omega) = -(1/\pi) \text{Im} G_0(s, \mathbf{k}, \omega) = \delta(\omega - \xi_{s\mathbf{k}})$. Electron-electron interactions cause scattering of the non-interacting excitations resulting in the broadening of the delta function peaks and shifting of spectral weight. This is incorporated through the modification of the interacting Green function by a self energy term, $G^{-1}(s, \mathbf{k}, \omega) = G_0^{-1}(s, \mathbf{k}, \omega) - \Sigma_s(\mathbf{k}, \omega)$ and the corresponding spectral function is given by

$$A(s, \mathbf{k}, \omega) = -\frac{1}{\pi} \frac{\Sigma_s''(\mathbf{k}, \omega)}{[\omega - \xi_{s\mathbf{k}} - \Sigma_s'(\mathbf{k}, \omega)]^2 + [\Sigma_s''(\mathbf{k}, \omega)]^2} \quad (1)$$

where $\Sigma_s(\mathbf{k}, \omega + i0^+) = \Sigma_s'(\mathbf{k}, \omega) + i\Sigma_s''(\mathbf{k}, \omega)$. Thus the imaginary part of self-energy incorporates the broadening of the spectral function peak while the real part determines the shift in the energy dispersion, especially near the Fermi surface.

We calculate the self-energy and hence the spectral function of a doped BLG system within the dynamical RPA at zero temperature. Using Matsubara frequencies, the self-energy can be written as

$$\Sigma(s, \mathbf{k}, i\omega) = -\frac{g}{\beta} \sum_{s', i\omega'} \int d^2\mathbf{q} \frac{V_c(\mathbf{q})}{\epsilon(\mathbf{q}, i\omega')} G_0(s', \mathbf{k} - \mathbf{q}, i\omega - i\omega') F_{ss'}(\mathbf{k}, \mathbf{q}) \quad (2)$$

where $i\omega$ and $i\omega'$ are respectively fermionic and bosonic Matsubara frequencies. Here $V_c(q) = 2\pi e^2 / (\kappa q)$ is the 2D bare Coulomb potential (κ being the background dielectric constant). Using E_F as units of energy and k_F as units of momentum, the strength of the interaction can be written in terms of the dimensionless coupling parameter $r_s = e^2 g m / (\kappa k_F)$. Unlike SLG (but similar to 2DEG), r_s in BLG can be tuned by changing the density of carriers ($r_s \sim n^{-1/2}$) and we will present our results as a function of r_s rather than the density. The dielectric function $\epsilon(\mathbf{q}, \omega)$, which incorporates the effects of dynamic screening, was calculated analytically in Ref. 7. Finally, the chirality of the bands is encoded in the overlap vertex factor $F_{ss'}(\mathbf{k}, \mathbf{q}) = (1 + ss' \cos 2\theta) / 2$, where θ is the angle between \mathbf{k} and $\mathbf{k} + \mathbf{q}$.

Although it is customary to separate the self-energy into an exchange and a correlation contribution, we prefer to work with the full expression since the exchange contribution, by itself, is divergent due to presence of the filled Fermi sea in the valence band. The total contribution, however, is free of this divergence, showing that the use of the dynamically screened interaction is crucial in calculating the single particle spectral properties of BLG. It is important to emphasize that our dynamical RPA self-energy calculation is theoretically well-defined and does not involve any arbitrary infrared or ultraviolet regularization through arbitrary momentum cut-offs.

Spectral function: With no loss of generality, we assume the BLG chemical potential to be in the conduction band. Since we are interested in the low energy properties around the Fermi surface, we will focus on $A(+, \mathbf{k}, \omega)$ and drop the index s from now on. In the left hand column of Fig. 1 we

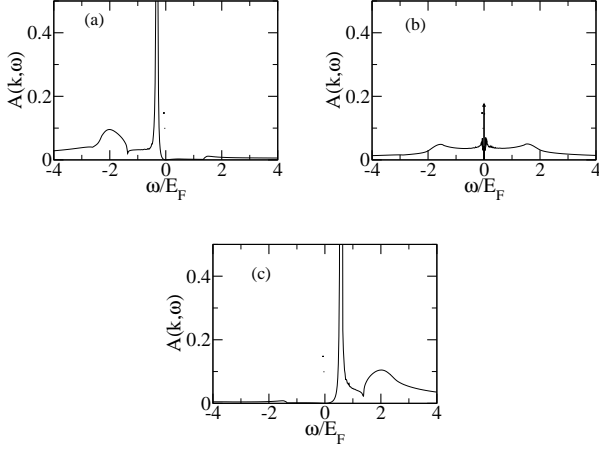


FIG. 2: Single particle spectral function for the wave vectors, (a) $k = 0.75k_F$, (b) $k = k_F$ and (c) $k = 1.25k_F$ for a system characterized by $r_s = 7$. The low energy quasiparticle peaks are accompanied by plasmaron features away from $k = k_F$.

plot the calculated real and imaginary parts of the self-energy for three wavevectors, (a) $k = 0.75k_F$ (b) $k = k_F$ and (c) $k = 1.25k_F$, in a system characterized by $r_s = 3$, corresponding to carrier density $n = 3 \times 10^{12} \text{cm}^{-2}$ for SiO_2 substrate. The self-energy has two distinct observable structures, coming from scattering off plasmon collective modes (plasmarons) and the continuum of particle hole excitations. In the imaginary part of the self-energy, the plasmon contribution leads to distinct logarithmic singularities away from $k = k_F$. These singularities are accompanied by jumps in the real part of the self-energy. The continuum contribution leads to an increasing background and dominates the self-energy at large values of ω . In the right hand column of Fig. 1, we plot the corresponding BLG spectral function. We also show the spectral function for a larger value of $r_s = 7$ (lower density of $n = 6 \times 10^{11} \text{cm}^{-2}$) in Fig. 2. The spectral functions at these two values of r_s show qualitatively similar features, although for the larger value of r_s , the incoherent background part of the spectral weight is spread over a larger energy. The prominent feature of the spectral function, manifesting its Fermi liquid characteristics, consists of a quasiparticle peak which disperses across the Fermi energy as the wave-vector goes across the Fermi surface. The quasiparticle peak is broadened for wavevectors away from $k = k_F$. At $k = k_F$, the spectral function has a delta function peak at the Fermi energy with a weight $Z \sim 0.4$ for $r_s = 3$ and $Z \sim 0.28$ for $r_s = 7$. This is the classic Fermi liquid behavior of an interacting electron system. Away from the Fermi wavevector, the spectral function consists of a double peaked structure. The second peak, arising from the dressing of the quasiparticles by the plasmon modes, is often referred to in the literature as a plasmaron. In SLG systems, these satellite bands have already been observed in ARPES experiments [3], and our current work shows that both the quasiparticle peak and the

plasmaron should be manifestly observable in BLG as well.

Landau's great insight in to the theory of interacting Fermi systems was that due to phase space constraints arising from Pauli blocking, the imaginary part of the self energy vanishes rapidly as one approaches the Fermi surface and weakly interacting quasiparticles form the low energy elementary excitations of the system. In a 2DEG, at low energies, the width of the quasiparticle peak $\Gamma_{\mathbf{k}} = \text{Im}\Sigma(\mathbf{k}, \xi_{\mathbf{k}}) \sim (\xi_{\mathbf{k}}^2/E_F) \ln(\xi_{\mathbf{k}}/E_F)$. This ensures that the spectral function has a delta function peak at the Fermi surface with a finite weight $Z < 1$. For BLG, we analytically find that the leading order quasiparticle scattering rate follows the same asymptotic form, as shown in Fig. 3(a). In fact this can be analytically shown to be true for arbitrarily large values of r_s . Thus the system remains a Fermi liquid for arbitrarily small densities. Several authors [5] have recently shown that the strictly undoped zero density neutral graphene is a non Fermi liquid with a vanishing Z factor and $\text{Im}\Sigma(k, \omega) \sim \omega$. However this non Fermi liquid behaviour relies on two peculiar features of undoped BLG : (a) a quadratic dispersion around a single Fermi point and (b) the interband scattering contribution persisting upto $\omega = 0$. Both these conditions are violated at any finite carrier density: the dispersion becomes linear around the Fermi surface and the interband scattering contribution is cut-off at a scale of E_F . The low energy quasiparticle width is in fact dominated by forward scattering from intraband particle-hole continuum and follows the usual Fermi liquid form. In the renormalization group language, the chemical potential is a relevant perturbation (even at the tree level) and thus the non Fermi liquid fixed point is unstable to arbitrarily small densities. We therefore conclude that the BLG is always a Fermi liquid.

Thus, for the doped BLG near the Fermi surface, the spectral function can be written as

$$A(\mathbf{k}, \omega) = Z_k \delta(\omega - v_F k + \mu) + A^{\text{inc}}(\mathbf{k}, \omega) \quad (3)$$

where μ is the chemical potential of the system, v_F is the slope of the dispersion, Z is the quasiparticle spectral weight and A^{inc} the non-singular incoherent part of the spectral function. The effective mass of the quasiparticles, which enters into low temperature thermodynamic properties like specific heat, is defined as $m^* = k_F/v_F$. The self-energy at low energies thus contains important information about the quasiparticle dispersion, broadening and spectral weight.

Quasiparticle spectral weight: As mentioned before, phase space restrictions associated with the fermionic Pauli principle lead to sharply defined quasiparticles near the Fermi surface in the interacting system producing the one-to-one Fermi liquid correspondence with the non-interacting Fermi gas. In BLG, the imaginary part of the self-energy at $k = k_F$ vanishes as $\omega^2 \ln \omega$ as one approaches the Fermi energy and exactly at the Fermi surface, the spectral function has a delta function peak with a weight $Z \leq 1$. This leads to a discontinuity in the momentum distribution at the Fermi surface (at $T = 0$) with the magnitude of the discontinuity given by Z . In terms of the

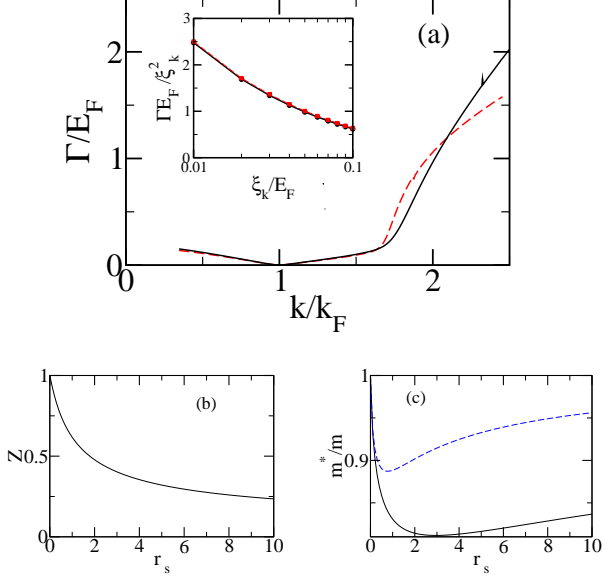


FIG. 3: (Color online): (a) Width of the quasiparticle peaks, $\Gamma_{\mathbf{k}} = Im\Sigma(\mathbf{k}, \xi_{\mathbf{k}})$, as a function of k/k_F for two different values of r_s . The red dashed line is for $r_s = 3$ and the thick black line is for $r_s = 7$. Inset: The low energy part of $\Gamma_{\mathbf{k}}/\xi_{\mathbf{k}}^2$ as a function of $\xi_{\mathbf{k}}$ for $r_s = 3$ and $r_s = 7$. The x-axis is logarithmic and the linear plot shows the $\omega^2 \ln \omega$ scaling of the quasiparticle width. (b) The quasiparticle weight, Z , as a function of r_s . (c) The effective mass m^* as a function of r_s . In (b) the thick black line is obtained from the on-shell approximation whereas the blue dashed line is the self-consistent solution.

self energy the quasiparticle spectral weight is given by

$$Z^{-1} = 1 - \frac{\partial \Sigma'(k_F, \omega)}{\partial \omega} \Big|_{k_F, E_F}. \quad (4)$$

In Fig. 3(a), we plot the BLG quasiparticle weight as a function of r_s . The quasiparticle weight decreases monotonically with increasing r_s (decreasing density), as stronger interactions shift spectral weight away from the quasiparticle pole. For very large r_s , Z eventually slowly approaches zero asymptotically with the system remaining a Fermi liquid for all r_s except the zero density infinite r_s singular point.

The energy dispersion of the quasiparticle excitations can be extracted either from the self-consistent solution of Dyson's equation (often called the off-shell approximation)

$$\omega_k - \xi_{\mathbf{k}} - \Sigma'(\mathbf{k}, \omega_k) = 0 \quad (5)$$

or from the on-shell approximation (OSA)

$$\omega_k - \xi_{\mathbf{k}} - \Sigma'(\mathbf{k}, \xi_k) = 0 \quad (6)$$

It is clear that if the self-energy is calculated exactly, the Dyson equation must be solved self-consistently. However the RPA involves a single-loop leading-order approximation

in the dynamically screened Coulomb interaction and as such, the dispersion should be calculated within the OSA to get consistent results within RPA [8]. However, since the use of the off-shell approximation is found in various places in the literature, we present our results both within the OSA and the off-shell Dyson equation approximations. We find that the interaction effects for the off-shell approximation are smaller than those for the OSA. We believe that experimental measurements of effective mass and/or the Z -factor compared with our theory could shed light on the important question of the relative validity of on-shell versus off-shell approximation.

The effective mass (m^):* The slope of the quasiparticle dispersion around the Fermi surface determines the Fermi velocity v_F which can be written in terms of the effective mass of the Landau quasiparticles as $v_F = k_F/m^*$. The self consistent solution to the Dyson equation yields

$$\frac{m^*}{m_0} = \frac{Z^{-1}}{1 + \frac{m_0}{k_F} \frac{\partial \Sigma'(k, \omega)}{\partial k} \Big|_{k_F, E_F}} \quad (7)$$

where Z is the quasiparticle weight. The on-shell approximation gives

$$\frac{m^*}{m_0} = \frac{1}{1 + \frac{m_0}{k_F} \frac{\partial \Sigma'(k, \omega)}{\partial k} \Big|_{k_F, E_F} + \frac{\partial \Sigma'(k, \omega)}{\partial \omega} \Big|_{k_F, E_F}} \quad (8)$$

The effective mass obtained from both calculations is plotted as a function of r_s in Fig. 3(b). We find that the effective mass at first decreases with increasing r_s and then exhibits a weak nonmonotonicity for larger r_s , where it tends to increase a bit, with the renormalized mass being always less than the bare band mass even for r_s as large as 10. This is very different from 2DEG and 3DEG systems where the effective mass renormalizes to values much larger than the bare mass for r_s larger than unity [8]. This prediction of our theory, which is somewhat counterintuitive (i.e. the renormalized mass being less than the bare mass even for strong interaction), is easily experimentally verifiable. We note that the BLG effective mass renormalization is small (only of the order of $\sim 20\%$ or less) in sharp contrast to 2DEG or 3DEG where the mass renormalization could be by a factor of 5 or more at larger r_s [8]. The relatively small BLG mass renormalization indicates a larger regime of validity for dynamical RPA in the chiral gapless BLG system compared with the standard 2DEG system. The maximum mass renormalization of $\sim 20\%$ also shows that the system remains a weakly interacting Fermi liquid upto a relatively large r_s .

Conclusion: We have calculated the effects of electron-electron interaction on the single particle spectral function of bilayer graphene within the random phase approximation. The spectral function shows a clear satellite plasmon peak in addition to the Landau quasiparticle peak near the Fermi surface. Thus, it should be possible to obtain information about collective plasmon excitations in the system by looking for these satellite peaks in ARPES data. Focusing on the low energy properties of the Landau quasiparticles, we have

calculated the quasiparticle weight and the effective mass of the Landau quasiparticles as a function of r_s . We show that inclusion of dynamic screening is crucial in obtaining these results. We also show that the presence of the valence band leads to relatively small renormalization in the low energy spectral properties, and thus the system remains a weakly interacting Fermi liquid upto relatively large values of r_s or relatively low densities. In addition to obtaining the quasiparticle spectral function, the effective mass renormalization, the inelastic scattering rate, and the quasiparticle renormalization factor, we have established the theoretical principle that doped BLG is always a Fermi liquid in contrast to undoped BLG.

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